

Local impurities in 2D Quantum Antiferromagnets

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The 2D quantum Heisenberg antiferromagnet at zero temperature with two kinds of locally frustrating defects - ferromagnetic bonds and impurity spins, is studied. An analytic approach is developed to investigate strong defect-environment couplings. Results for the local ground state properties are compared to numerical simulations and previous work.

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The two-dimensional Heisenberg antiferromagnet (HAFM) has attracted a lot of attention recently, mainly because of its relevance to the physics of the high- T_c materials. Doping with holes, which is crucial for the superconducting properties, leads to frustration of the spins and ultimately to destruction of antiferromagnetic (AFM) order. While the holes generally can hop, the extreme limit of static holes, acting as locally frustrating defects, is believed to describe some of the physics [1,2].

We study the Hamiltonian:

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - K \vec{S}_1 \cdot \vec{S}_2 + L \vec{S}_0 \cdot (\vec{S}_1 + \vec{S}_2). \quad (1)$$

The first term is the HAFM on a square lattice with nearest neighbor interactions (we set $J = 1$ from now on). The second and third term describe, respectively, a ferromagnetic bond (FMB) of strength $K \geq 0$, connecting the neighbor sites 1 and 2, and a quantum impurity spin \vec{S}_0 , coupled to those two sites. All the spins are 1/2. Without the two perturbations, the HAFM is known to have an ordered two-sublattice ground state [2]. Both additional terms lead to local frustration and thus influence the AFM order in the neighborhood of the defect.

First, we reconsider the case of a FMB in an AFM environment ($L = 0, K \neq 0$), previously studied in Ref.[3] in the linear spin-wave approximation (LSWA). Since the perturbation is local, it is natural first to solve the problem of the two spins, connected by the bond, and then take into account their interaction with the AFM environment (spin waves). Technically, we compute the two-particle Green's function of the spins 1 and 2. Details can be found in Ref.[5]. The interaction Hamiltonian is,

$$H_{int} = \frac{1}{2} \{ S_1^+ \sum_{nn1} a_i^+ + S_2^+ \sum_{nn2} b_j + h.c. \}, \quad (2)$$

which represents the transverse part of the interaction of the spins 1 and 2 with their neighbors (the sums stand for the three nearest neighbors only, excluding the other spin, connected by the bond). Here a and b are the Holstein-Primakoff operators on the two sublattices [2]. The full Hamiltonian is a sum of H_{int} , the Ising part of the interactions in H_{int} and the usual free spin wave term. Since the defect disturbs the AFM order away from it very weakly, one can treat the Ising terms in mean-field, by replacing $S_1^z S_i^z \rightarrow S_1^z \langle S_i^z \rangle$, where i is any neighbor of 1, and similarly for the other spin. We take $\langle S_i^z \rangle = 0.303$, which is the magnetization of the clean HAFM in LSWA [2].

We have developed a perturbation theory for H_{int} , keeping only the leading (one-loop) contributions to the self-energy [5]. For the unperturbed case ($K = 0$), this approach gives $M \equiv \langle S_1^z \rangle = 0.316$, a slightly higher value than the LSWA. Our results for different values of K are summarized in Fig.1., where the correlation function $C(1, 2) = \langle \vec{S}_1 \cdot \vec{S}_2 \rangle$ is also plotted. Additionally, we have performed numerical simulations, based on exact

diagonalization on small clusters, with very similar results, which, for lack of space, are not presented on the figure. The numerical procedure we have used differs from the one in previous studies [4]. In the spirit of our analytic approach, a staggered magnetic field of magnitude $|h| = 0.303$ was applied to the spins on the boundary of the cluster (typically containing $N = 18$ spins). An additional advantage of using such a field is that it breaks the sublattice symmetry, thus allowing for a non-zero staggered magnetization.

The behavior of the local magnetization within our approach is clearly quite different from the LSWA result. Up to $K = 1$ the two curves follow each other closely, both predicting a slight increase of M at that value (corresponding to a missing bond). For larger K the magnetization in LSWA drops sharply, eventually goes through 0 and then diverges at $K = 2$, signaling an instability, which is related to a local triplet formation. Of course, one expects to be below the range of validity of the LSWA even below $K = 2$, since the number of generated spin waves is large and interactions between them become important.

Our result for the magnetization clearly shows that the range of validity of LSWA is limited to small values of K , up to $K = 1$. Beyond this point the local magnetization decreases slowly and stays non-zero even for large K . On the other hand, the correlations across the FMB change from AFM to ferromagnetic at $K \approx 2.1$. One can show that it is the transverse (in plane) part of the correlator, which changes sign, while the Ising part shows AFM correlations for all K [5]. With increasing K the transverse part increases and the Ising one decreases (in magnitude), but remains non-zero, which is consistent with a finite magnetization. To conclude, our approach naturally describes the local triplet formation at $K \approx 2$; moreover, it can be used far beyond this point.

Next, we discuss the case $L \neq 0, K = 1$, corresponding to a quantum impurity spin in an AFM background (the bond between the spins, interacting with the impurity, is subtracted). We consider the three-particle Green's function (of the impurity spin and its neighbors), and apply the method described above [5]. The results are summarized in Fig.2. Again, only our analytic results are presented; the numerical simulations follow closely the plotted curves. The magnetization is defined in the usual way: $M(i) = \langle S_i^z \rangle$. It is assumed that for $L = 0$ the spin \vec{S}_1 belongs to sublattice A (spin up), \vec{S}_2 - to sublattice B (spin down) and $S_0^z = 1/2$. For ferromagnetic coupling $L \leq 0$, all correlations become ferromagnetic for sufficiently large $|L|$. However, this is not accompanied by a change in the ground state, since all the three spins have a non-zero magnetization (Fig.2.). This was already pointed out in Ref.[4]. For antiferromagnetic coupling $L \geq 0$, the spins 0 and 2 change their direction at $L \approx 2.3$ ($M(0)$ and $M(2)$ change sign). Naturally, the magnetization on site 1 increases at this point, since \vec{S}_1 is no longer frustrated. This local ground state phase transition has already been observed numerically in Ref.[4] for a finite size system of $N=18+1$ spins. However, a finite jump in all correlation functions, as well as magnetizations was reported there, while we observe a continuous behavior. We believe the discontinuity to be a finite size effect.

In summary, we have developed a technique, which allows us to study the effects of locally frustrating perturbations in 2D quantum antiferromagnets for any strength of the coupling. For an isolated FMB we find that the local magnetization does not vanish even for strong coupling - a result, suggesting that the previously used LSWA leads to qualitatively wrong behavior, and its region of validity is limited to small coupling only. We also study frustration, produced by a quantum impurity spin, coupled symmetrically to the two sublattices and describe the local ground state transition which we find in this case for antiferromagnetic sign of the coupling.

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FIGURE CAPTIONS

Fig.1. The magnetization M (solid line) and the correlation function $C(1, 2)$ (long dashed line) as a function of the ferromagnetic bond's strength. The short dashed line is the magnetization, calculated in LSWA [3].

Fig.2. Local magnetization at the impurity and the neighbor sites versus interaction strength.



